Supporting Information for

Unprecedented multicomponent organocatalytic synthesis of propargylic esters via CO_2 activation

by

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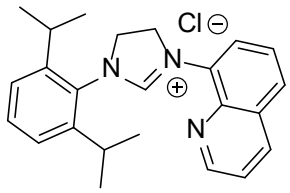
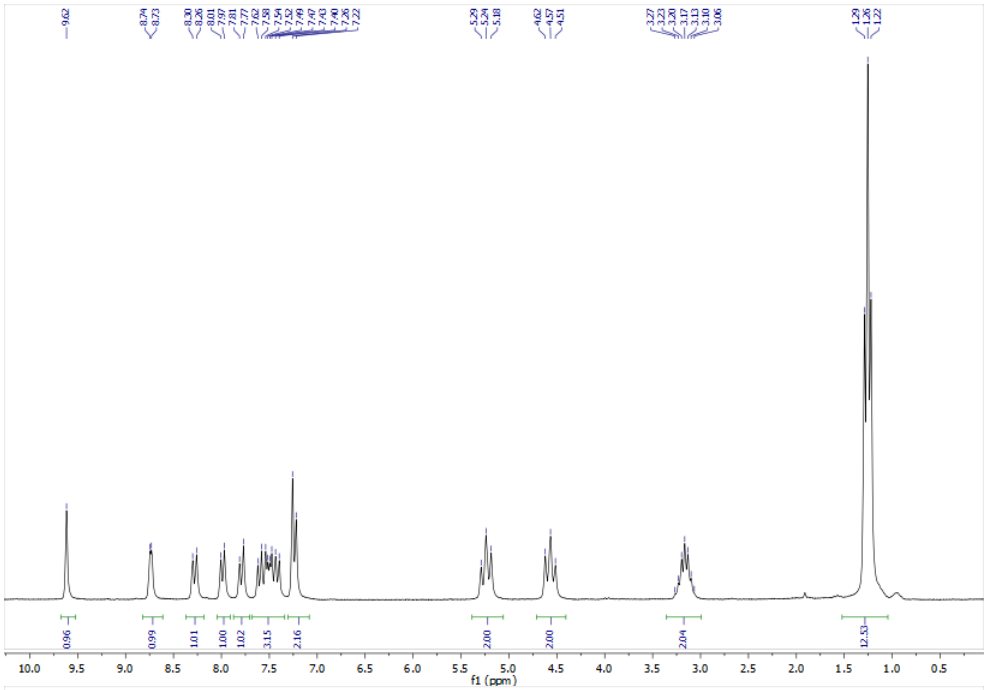
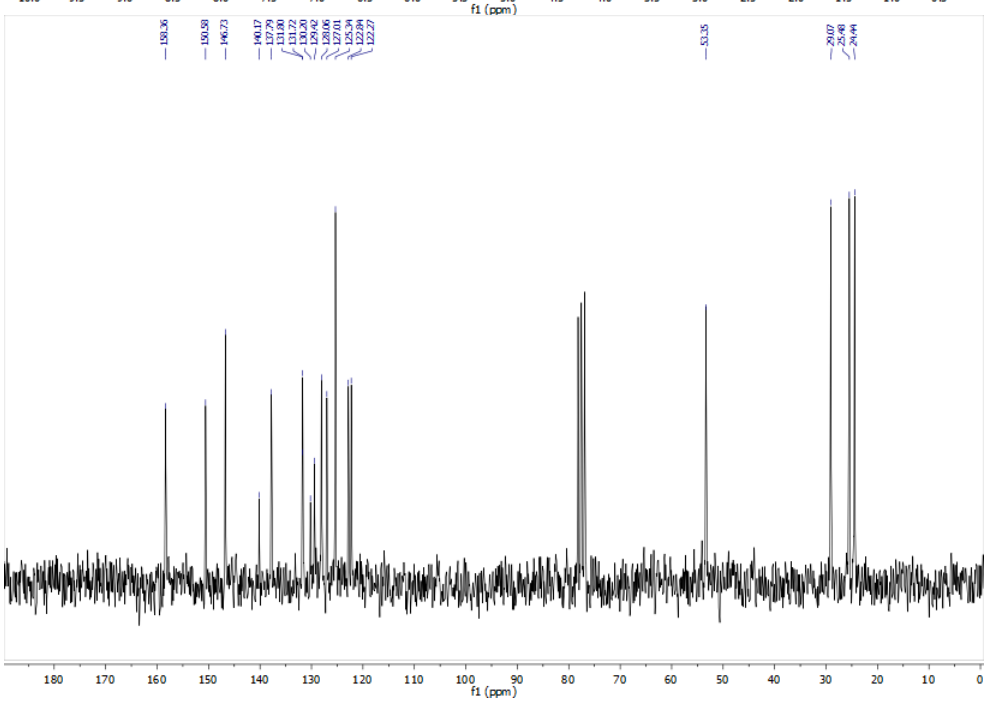
NMR spectra:

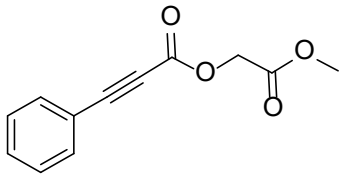
- **1-(2,6-Diisopropylphenyl)-3-(quinolin-8-yl)-4,5-dihydro-1H-imidazol-3-ium chloride.**

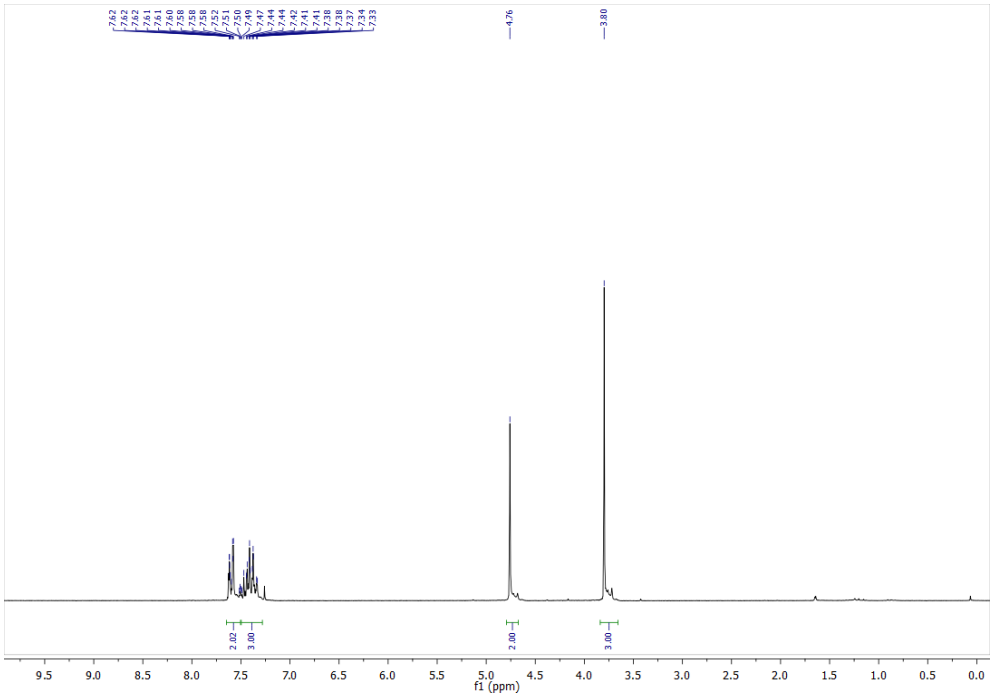


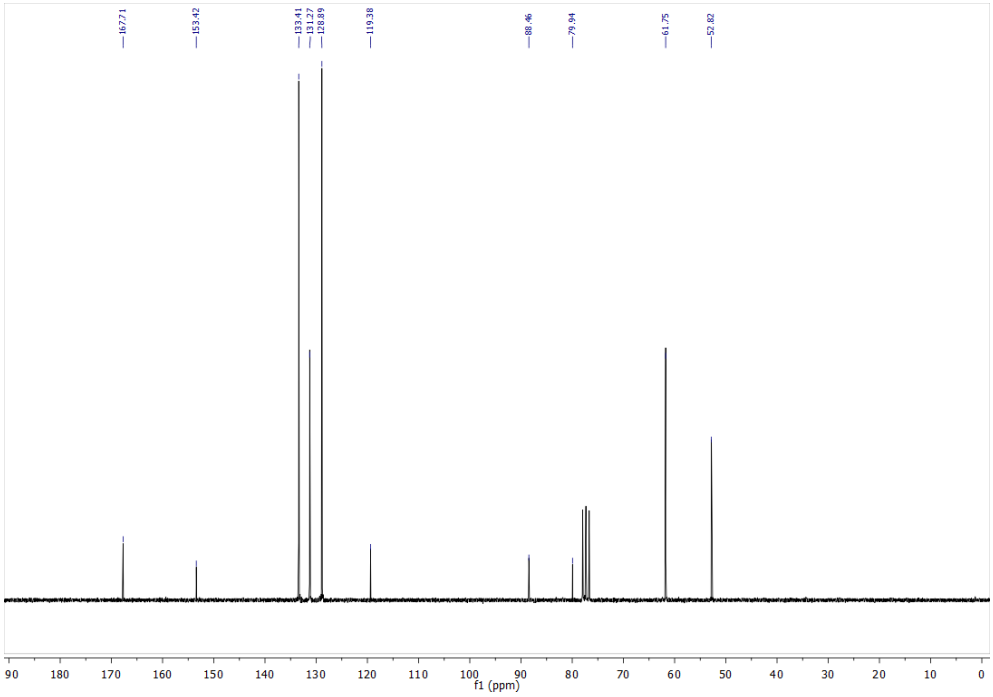




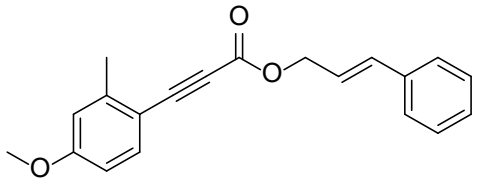
- **2-Methoxy-2-oxoethyl 3-phenylpropiolate.**

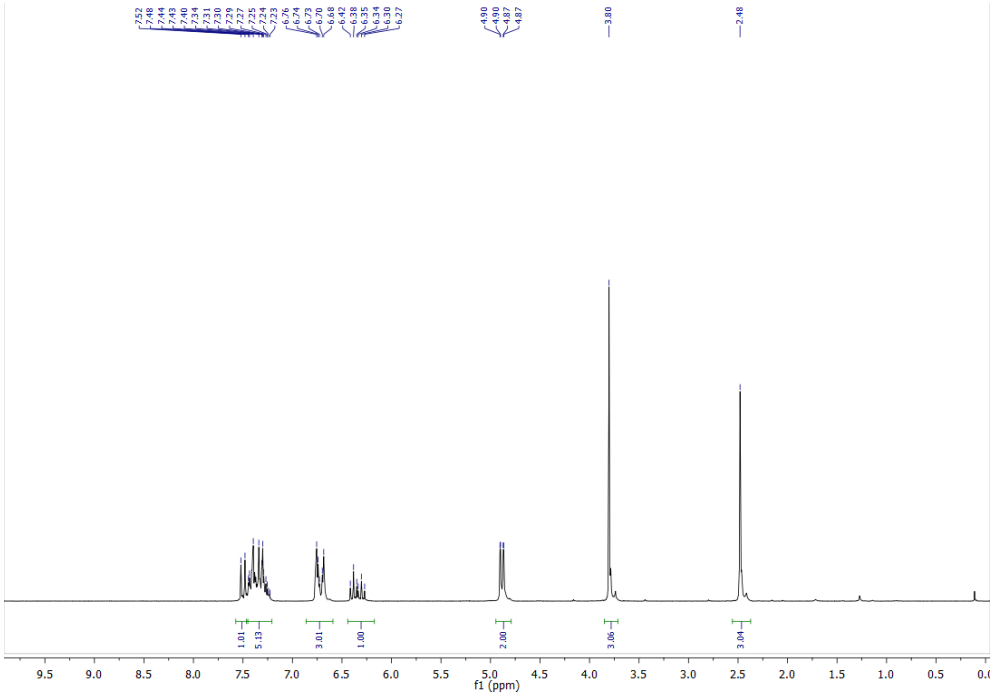


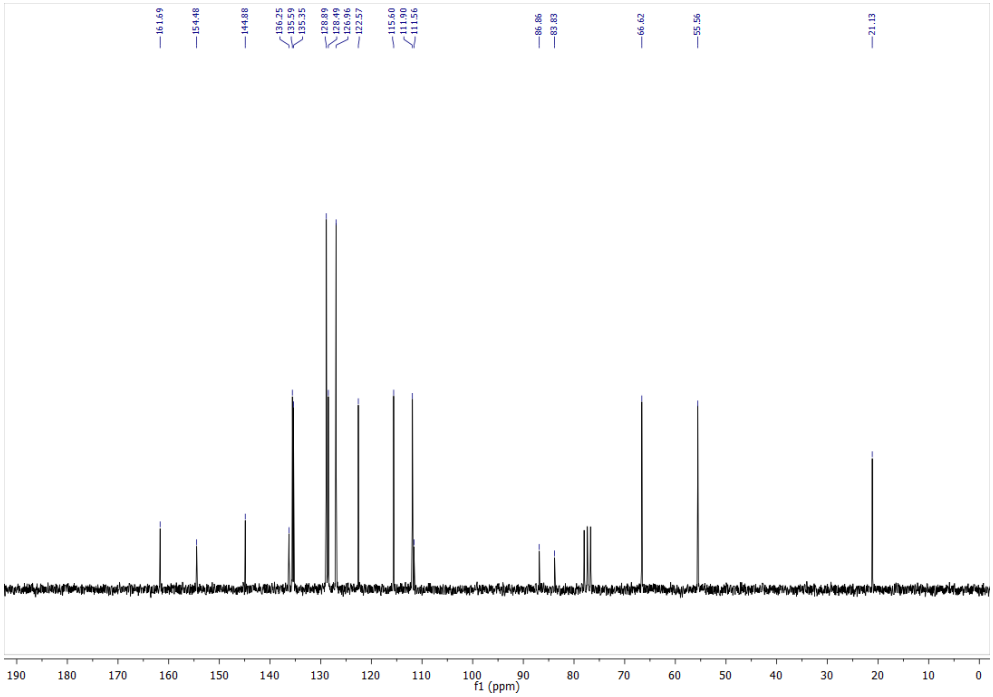




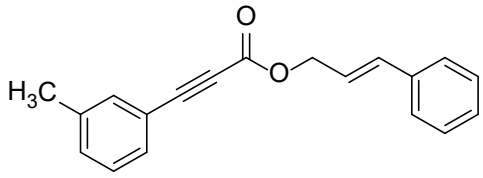
- **Cinnamyl 3-(4-methoxy-2-methylphenyl)propiolate.**

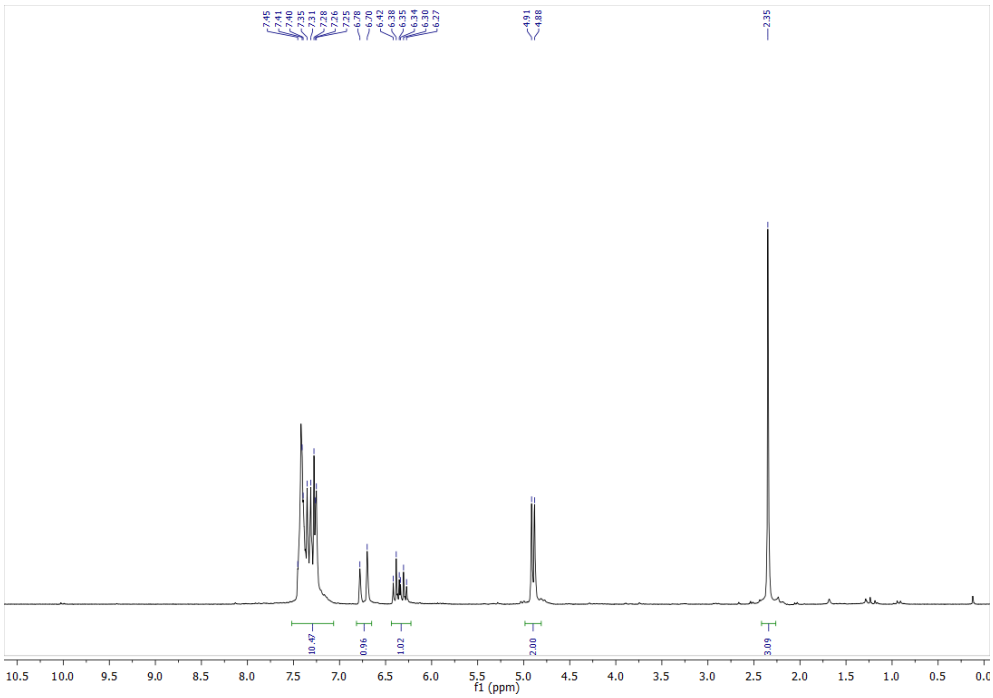


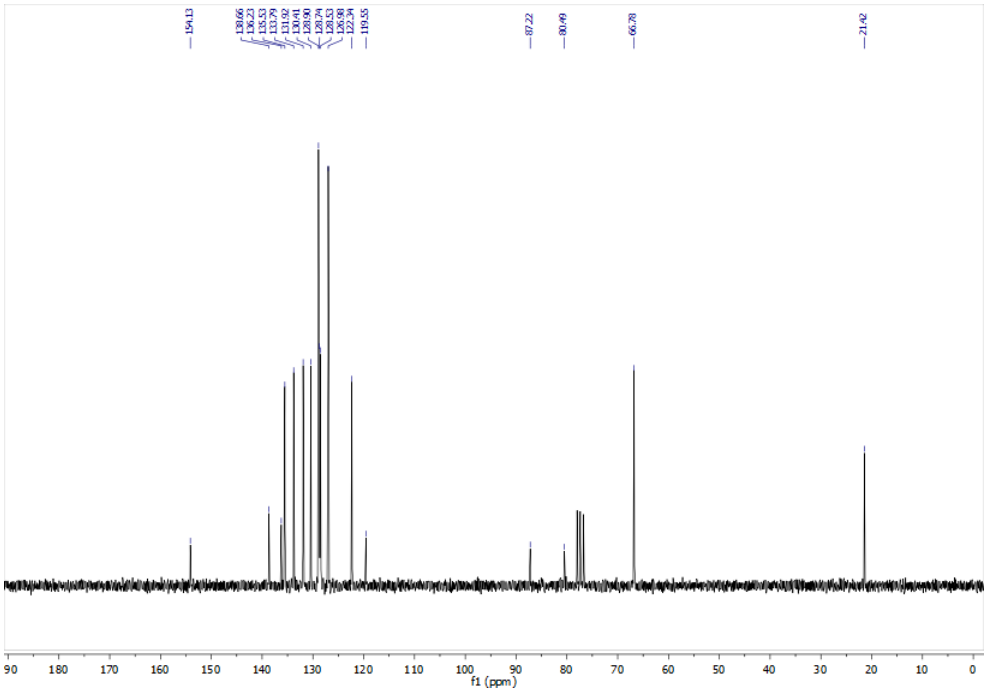




- **Cinnamyl 3-(m-tolyl)propiolate.**







Computational Methods:

All reported structures were optimized at Density Functional Theory level by using the B3LYP[1] functional as implemented in Gaussian 09.[2] Optimizations were carried out with the 6-31G(d,p) basis set. The reported energy values correspond to Gibbs Free energies, including single point refinements at M06-2X/def2tzvpp[3] level of theory in a solvent model (IEFPCM, dimethylformamide)[4] on the previously optimized structures. The critical stationary points were characterized by frequency calculations in order to verify that they have the right number of imaginary frequencies, and the intrinsic reaction coordinates (IRC)[5] were followed to verify the energy profiles connecting the key transition structures to the correct associated local minima.

[1] (a) C. Lee, W. Yang, R.G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789; (b) A. D. Becke, *J. Chem. Phys*. **1993**, *98*, 5648-5652; (c) W. Kohn, A. D. Becke, R. G. Parr, *J. Phys. Chem.* **1996**, *100*, 12974-12980.

[2] Gaussian 09, Revision D.01; M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.

[3] Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215-241.

[4] (a) E. Cancès, B. Mennucci, J. Tomasi, *J. Chem. Phys*. **1997**, *107*, 3032–3047; (b) M. Cossi, V. Barone, B. Mennuci, J. Tomasi, *Chem. Phys. Lett.* **1998**, *286*, 253–260; (c) J. Tomasi, B. Mennucci, E. Cancès, *J. Mol. Struct*. (Theochem), **1999**, *464*, 211–226.

[5] C. Gonzalez, H. B. Schlegel, *J. Phys. Chem*. **1990**, *94*, 5523–5527.

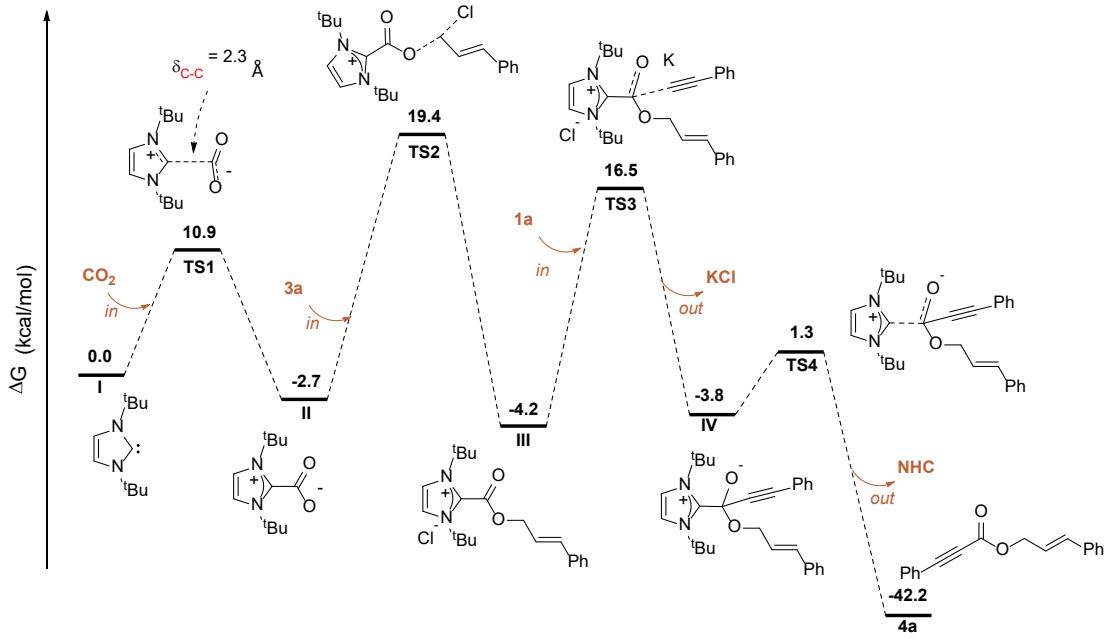


Figure S1. Energy profile for the catalytic cycle of the reaction between **1a**, **3a**, and CO_2.

Cartesian Coordinates of the computed structures in Figure S1

I

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -540.394217 Hartrees

Standard orientation:

Atomic Type	X	Y	Z
N	-0.943400	-0.004600	0.000000
C	-0.872600	-1.268600	0.000000
C	0.400500	-1.677100	0.000000
N	1.193600	-0.690300	0.000000
C	0.427000	0.527200	0.000000
C	-2.179200	0.791600	0.000000
C	2.661200	-0.774900	0.000000
C	-3.384100	-0.140000	0.000000
C	-2.216900	1.669100	1.244200
C	-2.216900	1.670000	-1.243600
C	3.086100	-2.237400	0.000000
C	3.208500	-0.088000	-1.244200
C	3.209100	-0.087300	1.243600
H	-1.742800	-1.941400	0.000000
H	0.716700	-2.730700	0.000000
H	-4.319700	0.462800	0.000000
H	-3.356500	-0.781300	-0.909300
H	-3.356500	-0.781900	0.908800
H	-3.152200	2.272400	1.245200

H	-1.336700	2.350300	1.243900
H	-2.189300	1.026300	2.152400
H	-1.299900	1.495400	-1.849700
H	-3.115300	1.416000	-1.849500
H	-2.263100	2.739900	-0.940600
H	4.197300	-2.301500	0.000000
H	2.686100	-2.739400	0.909300
H	2.685700	-2.739900	-0.908800
H	4.319700	-0.151500	-1.245200
H	2.898500	0.981000	-1.243900
H	2.807600	-0.591200	-2.152400
H	2.365200	0.311800	1.849700
H	3.785400	-0.821800	1.849500
H	3.876600	0.750100	0.940600

CO_2

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -188.608132 Hartrees

Standard orientation:

Atomic Type	X	Y	Z
O	1.023710	0.067050	-0.054640
C	2.220710	0.067050	-0.054640
O	3.417710	0.067050	-0.054640

II

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -729.008964 Hartrees

Standard orientation:

Atomic Type	X	Y	Z
N	-0.949535	0.001162	-0.036720
C	-0.953085	-1.380112	0.015784
C	0.334283	-1.785381	0.061942
N	1.124961	-0.651754	0.043053
C	0.324708	0.425092	-0.018101
C	-2.188749	0.856498	-0.023621
C	2.630261	-0.664420	0.006174
C	-3.369975	-0.001090	-0.478893
C	-2.409934	1.343339	1.409015
C	-2.024159	2.029145	-0.994014
C	3.112700	-2.019631	0.524512
C	3.067512	-0.467488	-1.445863
C	3.184059	0.438759	0.911828
O	1.287679	2.248442	-1.137946
C	0.791611	1.903265	-0.059868
O	0.601104	2.525397	0.990888
H	-1.853405	-1.964728	0.010454
H	0.735961	-2.779630	0.111973
H	-4.246347	0.643843	-0.544984
H	-3.190411	-0.438261	-1.463531

H	-3.602944	-0.793107	0.234071
H	-3.313283	1.956001	1.442494
H	-1.558569	1.938450	1.738358
H	-2.542249	0.493444	2.082339
H	-1.680344	1.682411	-1.970265
H	-2.998393	2.504006	-1.118289
H	-1.335579	2.781112	-0.614402
H	4.201451	-1.992082	0.571384
H	2.730917	-2.222854	1.527415
H	2.837221	-2.837570	-0.142550
H	4.158221	-0.486441	-1.496019
H	2.706312	0.490336	-1.819448
H	2.677549	-1.273025	-2.072138
H	2.718761	0.403761	1.898623
H	4.256137	0.273870	1.028140
H	3.046254	1.428743	0.482104

3a - Benzyl chloride

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -808.419964 Hartrees

Standard orientation:

Atomic Type	X	Y	Z
C	-2.374951	-0.804358	0.155950
C	-2.294862	-2.183608	-0.032038
C	-1.052410	-2.781973	-0.208096
C	0.101002	-2.004981	-0.196719
C	0.034718	-0.620093	-0.010105
C	-1.223917	-0.029855	0.167704
C	1.288414	0.151250	-0.011599
C	1.416955	1.469303	0.151418
C	2.743461	2.138513	0.156283
Cl	2.910419	3.238535	-1.294252
H	-3.340175	-0.332048	0.294427
H	-3.196103	-2.784620	-0.040083
H	-0.979169	-3.852913	-0.354490
H	1.069220	-2.474282	-0.334780
H	-1.308944	1.039917	0.316742
H	2.191427	-0.438434	-0.157459
H	0.555452	2.114154	0.293369
H	2.877107	2.794111	1.013302
H	3.564757	1.430083	0.089825

1a – Phenyl ethylene (K salt)

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -907.690444 Hartrees

Standard orientation:

Atomic Type	X	Y	Z
C	2.977298	1.060213	-0.281087
C	3.518660	-0.179613	0.050061

C	2.665171	-1.243487	0.332246
C	1.287308	-1.071423	0.284347
C	0.724539	0.172850	-0.048015
C	1.599901	1.235710	-0.329900
C	-0.699886	0.352533	-0.098017
C	-1.923865	0.506935	-0.140982
K	-4.694041	0.856554	-0.238242
H	3.631635	1.895624	-0.502699
H	4.592852	-0.315116	0.087766
H	3.074941	-2.213129	0.591209
H	0.626668	-1.901885	0.504631
H	1.182720	2.202133	-0.588017

III

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -1537.412149 Hartrees

Standard orientation:

Atomic Type	X	Y	Z
N	-2.171758	1.575409	0.278532
C	-3.295441	1.615495	1.070703
C	-3.941981	0.434384	0.924114
N	-3.218370	-0.329984	0.042955
C	-2.148478	0.380391	-0.327893
C	-1.149708	2.685941	0.184889
C	-3.597671	-1.726871	-0.394422
C	-1.830762	3.989600	0.602845
C	-0.001180	2.357607	1.138337
C	-0.662609	2.823308	-1.259883
C	-2.339115	-2.588162	-0.538762
C	-4.482242	-2.329725	0.697176
C	-4.361168	-1.608322	-1.713036
O	-1.413762	-0.166172	-2.519054
C	-1.143565	-0.068168	-1.355156
O	0.022047	-0.322723	-0.800150
C	6.128877	-1.284309	1.315067
C	7.169767	-0.438571	0.933903
C	6.978770	0.459990	-0.109596
C	5.753605	0.512257	-0.765742
C	4.700893	-0.329332	-0.391823
C	4.907243	-1.232373	0.659465
C	3.423814	-0.224831	-1.117639
C	2.311275	-0.919909	-0.879445
C	1.081125	-0.754168	-1.701897
Cl	-1.335693	-1.220951	2.770636
H	-3.554329	2.465532	1.672778
H	-4.843952	0.088474	1.391924
H	-1.117761	4.800255	0.453611
H	-2.714025	4.191237	-0.006437
H	-2.105868	3.990809	1.657896
H	0.732490	3.164878	1.094266
H	0.485910	1.423090	0.859468

H	-0.367590	2.273543	2.163051
H	-1.498624	2.843852	-1.961418
H	-0.121624	3.766021	-1.344402
H	0.036633	2.037274	-1.542872
H	-2.651646	-3.632069	-0.579184
H	-1.800002	-2.387939	-1.464201
H	-1.684925	-2.451554	0.324433
H	-4.681234	-3.367957	0.431451
H	-5.445975	-1.824937	0.774220
H	-3.968729	-2.304183	1.660787
H	-5.258492	-0.999637	-1.584459
H	-3.733702	-1.162431	-2.485730
H	-4.661974	-2.606162	-2.037818
H	6.272203	-1.987896	2.126383
H	8.122313	-0.483451	1.447894
H	7.781769	1.120498	-0.413832
H	5.606572	1.214308	-1.579513
H	4.112648	-1.900760	0.968753
H	3.413916	0.498902	-1.930384
H	2.251227	-1.651706	-0.079826
H	1.202273	-0.002080	-2.483560
H	0.755220	-1.691953	-2.158090

4a

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -844.476432 Hartrees

Standard orientation:

Atomic Type	X	Y	Z
C	-4.007331	-2.373191	0.437706
C	-5.240258	-2.729584	-0.103343
C	-5.905698	-1.860553	-0.964555
C	-5.342373	-0.634241	-1.287989
C	-4.102573	-0.272991	-0.745032
C	-3.435594	-1.148946	0.121052
C	-3.519133	0.989914	-1.076252
C	-3.025303	2.053062	-1.354303
O	-3.024127	4.101483	-2.494906
C	-2.485654	3.344680	-1.729338
O	-1.325720	3.583207	-1.119697
C	4.512728	5.469269	1.240815
C	4.573706	6.405146	2.272037
C	3.451695	7.169132	2.574057
C	2.276267	6.994007	1.851825
C	2.198392	6.049879	0.822548
C	3.339227	5.294950	0.520436
C	0.923032	5.889808	0.102861
C	0.602342	4.900237	-0.730236
C	-0.702782	4.847254	-1.448453
H	-3.491325	-3.050129	1.107108
H	-5.683128	-3.685965	0.146761
H	-6.864180	-2.139118	-1.384475
H	-5.850877	0.049033	-1.956743

H	-2.477589	-0.861710	0.536268
H	5.386709	4.878622	0.993249
H	5.492276	6.540558	2.830123
H	3.490839	7.903151	3.369981
H	1.402608	7.591937	2.088564
H	3.315674	4.576147	-0.290111
H	0.181820	6.662745	0.296410
H	1.290681	4.086114	-0.937576
H	-1.365913	5.660995	-1.150151
H	-0.569842	4.884837	-2.532542

KCl

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -1060.273147 Hartrees

Standard orientation:

Atomic Type	X	Y	Z
K	1.142490	-0.095020	0.019750
Cl	3.859330	-0.095020	0.019750

TS1

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -728.982965 Hartrees
Imaginary Frequency -208.4 cm^{-1}

Standard orientation:

Atomic Type	X	Y	Z
N	-1.070920	-0.761792	-0.036123
C	-0.674840	-2.088771	-0.022673
C	0.674554	-2.088830	0.022726
N	1.070754	-0.761887	0.035921
C	-0.000043	0.074138	-0.000164
C	-2.489139	-0.300650	-0.084006
C	2.489014	-0.300858	0.083575
C	-3.424645	-1.508799	-0.115549
C	-2.780330	0.523862	1.170976
C	-2.694956	0.523773	-1.355846
C	2.780007	0.523702	-1.171426
C	2.695141	0.523458	1.355433
C	3.424427	-1.509088	0.114848
H	-1.357488	-2.918008	-0.045565
H	1.357128	-2.918125	0.045769
H	-4.451695	-1.143039	-0.150229
H	-3.257588	-2.126038	-1.000735
H	-3.317673	-2.125977	0.778930
H	-3.820156	0.857087	1.154764
H	-2.133606	1.397557	1.232124
H	-2.624305	-0.085087	2.064555
H	-2.478765	-0.085193	-2.236794
H	-3.733549	0.856834	-1.410002

H	-2.045684	1.397557	-1.373141
H	3.819848	0.856887	-1.155385
H	2.623801	-0.085212	-2.064998
H	2.133294	1.397420	-1.232414
H	3.733789	0.856364	1.409472
H	2.478982	-0.085531	2.236374
H	2.045999	1.397331	1.372916
H	3.257600	-2.126299	1.000096
H	3.317105	-2.126270	-0.779587
H	4.451522	-1.143424	0.149200
O	0.038624	2.617114	-1.147480
C	0.000043	2.373185	0.000233
O	-0.038559	2.616645	1.148055

TS2

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -1537.384283 Hartrees
Imaginary Frequency -541.8 cm^{-1}

Standard orientation:

Atomic Type	X	Y	Z
N	3.332496	-0.366049	0.185381
C	3.960817	-1.568534	-0.066854
C	3.015183	-2.441248	-0.480202
N	1.806513	-1.775463	-0.477115
C	2.023371	-0.515037	-0.069887
C	4.023255	0.859617	0.731969
C	0.498583	-2.379790	-0.924575
C	5.523110	0.717791	0.471698
C	3.511704	2.111094	0.013158
C	3.752487	0.922098	2.235638
C	0.635996	-3.901560	-0.896708
C	-0.610567	-1.958714	0.039376
C	0.215388	-1.899988	-2.348663
O	0.588601	1.068769	-1.015175
C	0.968760	0.591781	0.084159
O	0.639987	0.890677	1.225966
H	5.016840	-1.714340	0.058236
H	3.113882	-3.471524	-0.765015
H	6.006680	1.637202	0.801552
H	5.963609	-0.102801	1.039332
H	5.733755	0.581424	-0.591133
H	4.177576	2.938056	0.262780
H	2.509949	2.392989	0.331920
H	3.522611	1.972590	-1.069418
H	4.139630	0.028019	2.728895
H	4.260745	1.794583	2.650908
H	2.683620	1.007125	2.429189
H	-0.338263	-4.327181	-1.137657
H	1.343957	-4.265784	-1.642352
H	0.930487	-4.258747	0.092312
H	-1.512607	-2.524196	-0.202874
H	-0.857931	-0.904358	-0.058902

H	-0.334109	-2.171600	1.074167
H	1.016523	-2.212478	-3.021942
H	-0.719957	-2.346406	-2.692182
H	0.123409	-0.814438	-2.377363
C	-5.219504	-1.443781	-0.263721
C	-5.328085	-2.048224	0.988620
C	-4.517926	-1.621205	2.035471
C	-3.600653	-0.597558	1.828906
C	-3.473185	0.008525	0.573258
C	-4.301597	-0.425188	-0.471715
C	-2.446999	1.037921	0.397356
C	-2.028294	1.555641	-0.768436
C	-0.926280	2.490913	-0.804452
Cl	-2.207472	4.572550	-0.800986
H	-5.855640	-1.768487	-1.078237
H	-6.045276	-2.844822	1.145595
H	-4.600281	-2.083786	3.011467
H	-2.965107	-0.265826	2.642981
H	-4.234812	0.038853	-1.448476
H	-1.938019	1.359605	1.303127
H	-2.457209	1.259784	-1.718919
H	-0.470368	2.820056	0.115091
H	-0.541808	2.860831	-1.736874

TS3

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -1384.811738 Hartrees
Imaginary Frequency -147.5 cm^{-1}

Standard orientation:

Atomic Type	X	Y	Z
N	0.986477	-2.046072	1.496427
C	1.835593	-3.127700	1.479345
C	2.065172	-3.462213	0.195002
N	1.359857	-2.594889	-0.603479
C	0.712445	-1.717551	0.205550
C	0.520828	-1.456922	2.828847
C	1.397757	-2.735148	-2.124629
C	1.175025	-2.248037	3.970484
C	1.003894	-0.010904	2.964909
C	-0.992102	-1.655084	2.970427
C	1.946923	-1.457975	-2.762482
C	2.365983	-3.869001	-2.486290
C	0.010341	-3.149596	-2.621601
O	-0.504846	-0.510431	-1.469361
C	-0.116588	-0.558430	-0.320149
O	-0.765980	0.074735	0.671712
C	-6.932633	0.853359	-1.741010
C	-7.951185	1.207778	-0.857793
C	-7.627236	1.693664	0.404330
C	-6.294198	1.819203	0.780353

C	-5.262501	1.455989	-0.091985
C	-5.602440	0.979022	-1.364823
C	-3.866974	1.590846	0.361801
C	-2.787217	1.081922	-0.233013
C	-1.403900	1.305098	0.292764
H	2.212826	-3.597509	2.364838
H	2.670647	-4.259093	-0.186842
H	0.834175	-1.792961	4.900603
H	0.867255	-3.294809	3.984511
H	2.263782	-2.180837	3.952225
H	0.644986	0.373193	3.922297
H	0.659504	0.633128	2.165211
H	2.096057	0.008555	2.975602
H	-1.227173	-2.720051	2.905904
H	-1.290243	-1.303117	3.960044
H	-1.562091	-1.115777	2.223436
H	1.975453	-1.613517	-3.843311
H	1.343524	-0.584973	-2.543344
H	2.966593	-1.280574	-2.413821
H	2.389916	-3.925172	-3.574667
H	2.031445	-4.839303	-2.115718
H	3.382902	-3.671067	-2.143392
H	-0.285893	-4.086649	-2.144202
H	-0.736576	-2.388469	-2.427906
H	0.070093	-3.321666	-3.698312
H	-7.177618	0.484825	-2.730109
H	-8.988202	1.111503	-1.156009
H	-8.411207	1.977341	1.096332
H	-6.044558	2.199559	1.765224
H	-4.823330	0.716626	-2.070794
H	-3.733080	2.157276	1.281844
H	-2.859896	0.483294	-1.135063
H	-0.760273	1.792895	-0.444882
H	-1.426262	1.905813	1.202833
C	5.317143	3.967474	0.802403
C	6.047802	4.129451	-0.372238
C	5.674336	3.424401	-1.513860
C	4.582098	2.566151	-1.483198
C	3.835590	2.392991	-0.306318
C	4.224324	3.110167	0.836915
C	2.706700	1.505309	-0.272241
C	1.744131	0.740105	-0.239288
H	5.600068	4.511543	1.696177
H	6.899532	4.798449	-0.397732
H	6.236748	3.543465	-2.432775
H	4.292199	2.018636	-2.372612
H	3.656299	2.985522	1.75169

IV

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -2445.109336 Hartrees

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-2.719347	-1.980033	-0.938175		
C	-3.424506	-3.020586	-0.371478		
C	-2.990295	-3.177803	0.891361		
N	-2.007780	-2.240350	1.121111		
C	-1.814570	-1.536852	-0.023744		
C	-3.089185	-1.511826	-2.345191		
C	-1.401503	-2.097559	2.513485		
C	-4.539316	-1.945838	-2.621012		
C	-3.070773	0.013994	-2.448912		
C	-2.183000	-2.199638	-3.366597		
C	-1.337253	-0.621175	2.911243		
C	-2.334364	-2.787332	3.519875		
C	-0.048578	-2.809227	2.546660		
O	0.380521	-0.698202	0.539261		
C	-0.641891	-0.491696	-0.231310		
O	-0.347060	-0.695459	-1.631891		
C	6.225414	0.114514	-0.612676		
C	6.757344	1.290270	-0.087272		
C	5.972295	2.438425	-0.042037		
C	4.663950	2.406952	-0.511696		
C	4.114319	1.229816	-1.035509		
C	4.920976	0.084162	-1.090025		
C	2.706931	1.230037	-1.475508		
C	1.954640	0.151842	-1.707427		
C	0.543443	0.240391	-2.209879		
H	-4.185534	-3.569021	-0.889463		
H	-3.321885	-3.878492	1.631229		
H	-4.842005	-1.484347	-3.560656		
H	-4.641950	-3.023286	-2.750137		
H	-5.219800	-1.603501	-1.838949		
H	-3.520715	0.284594	-3.405601		
H	-2.071623	0.429761	-2.414672		
H	-3.671121	0.458848	-1.652203		
H	-2.267885	-3.284675	-3.269338		
H	-2.517369	-1.922325	-4.368810		
H	-1.145731	-1.908221	-3.237276		
H	-1.051666	-0.568820	3.963700		
H	-0.610310	-0.076536	2.319419		
H	-2.322813	-0.160500	2.804138		
H	-1.936658	-2.583290	4.514203		
H	-2.357609	-3.871070	3.402422		
H	-3.350528	-2.390415	3.473002		
H	-0.186555	-3.879114	2.370886		
H	0.613773	-2.400252	1.790328		
H	0.391527	-2.681947	3.538728		
H	6.831103	-0.783093	-0.657724		
H	7.776784	1.311534	0.278518		
H	6.377902	3.359349	0.359731		
H	4.052883	3.302468	-0.470330		
H	4.527798	-0.839234	-1.498744		
H	2.249323	2.213208	-1.571496		
H	2.349581	-0.855157	-1.583655		

H	0.164470	1.263917	-2.092767
H	0.529168	0.002235	-3.278866
C	-2.782002	5.043819	2.011470
C	-3.314728	5.799162	0.969838
C	-3.309042	5.294814	-0.328134
C	-2.773968	4.039688	-0.587632
C	-2.234875	3.276414	0.456031
C	-2.243007	3.788849	1.759761
C	-1.685141	1.978849	0.191578
C	-1.244157	0.880576	-0.041878
H	-2.785705	5.433651	3.022134
H	-3.733199	6.778239	1.169040
H	-3.722907	5.880254	-1.140164
H	-2.767326	3.640028	-1.594819
H	-1.826278	3.195963	2.565292
Cl	3.610035	-3.018525	0.335705
K	2.697974	-0.336954	1.369794

TS4

G at M06-2X/def2tzvpp//M06-2X/6-311G** (SDD, Ir) (IEFPCM, DMF) = -1384.657364 Hartrees
Imaginary Frequency -208.4 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-3.190339	-1.016928	-0.906749		
C	-4.207111	-1.882936	-0.543878		
C	-4.031790	-2.170920	0.760547		
N	-2.910173	-1.478157	1.180654		
C	-2.351073	-0.800708	0.141528		
C	-3.188590	-0.358813	-2.252372		
C	-2.517619	-1.440421	2.626735		
C	-4.635629	0.033901	-2.588644		
C	-2.360091	0.923204	-2.220987		
C	-2.666720	-1.346560	-3.296841		
C	-1.736138	-0.161493	2.924105		
C	-3.800988	-1.410523	3.469819		
C	-1.710943	-2.695960	2.962976		
O	0.190755	-1.394335	0.886845		
C	-0.277076	-0.658832	0.022700		
O	-0.268395	-1.112633	-1.307635		
C	6.019715	-2.977877	0.036821		
C	6.951682	-2.053987	0.506848		
C	6.673136	-0.694197	0.420248		
C	5.469746	-0.263753	-0.128126		
C	4.520827	-1.180545	-0.593786		
C	4.819219	-2.547153	-0.511052		
C	3.253648	-0.673965	-1.149180		
C	2.160546	-1.390324	-1.412250		
C	0.929973	-0.794171	-2.023278		

H	-4.973510	-2.213318	-1.221111
H	-4.622040	-2.791623	1.409381
H	-4.629613	0.620584	-3.508436
H	-5.277186	-0.830883	-2.759816
H	-5.066046	0.643573	-1.791148
H	-2.510879	1.449178	-3.165789
H	-1.301245	0.721618	-2.104780
H	-2.685231	1.573416	-1.405555
H	-3.299914	-2.236824	-3.329997
H	-2.687099	-0.877783	-4.283267
H	-1.647677	-1.645605	-3.059509
H	-1.583531	-0.098999	4.003555
H	-0.765269	-0.163090	2.439337
H	-2.304146	0.715677	2.605468
H	-3.522327	-1.244912	4.511490
H	-4.353273	-2.349944	3.428270
H	-4.457080	-0.596572	3.153442
H	-2.304311	-3.591400	2.760161
H	-0.797307	-2.725412	2.372963
H	-1.457183	-2.689795	4.025671
H	6.234182	-4.038656	0.091483
H	7.889002	-2.393546	0.930822
H	7.392739	0.032683	0.777868
H	5.255319	0.797713	-0.193903
H	4.114281	-3.278817	-0.888096
H	3.225340	0.398152	-1.337324
H	2.115914	-2.454930	-1.200660
H	1.039378	0.292632	-2.117761
H	0.760583	-1.208228	-3.020356
C	1.056807	5.317661	1.625489
C	0.714237	6.151215	0.563907
C	0.174486	5.609616	-0.600063
C	-0.024206	4.239407	-0.705362
C	0.319869	3.396372	0.359591
C	0.862924	3.946023	1.527789
C	0.111125	1.983180	0.248222
C	-0.095141	0.801087	0.134455
H	1.476582	5.737006	2.531709
H	0.867552	7.220587	0.643392
H	-0.092925	6.256125	-1.427010
H	-0.445139	3.809797	-1.606727
H	1.127819	3.291778	2.349428
